

## Research activity at a glance

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NAME Yoshihiro ASAI

AFFILIATION AIST, Japan

JOB Director, Research Center for Computational Design of Advanced Functional Materials in AIST

SUBJECTS Condensed matter theory, Chemical Physics, Computational Physics



## Photos

L.H.S. up: Y.A. R.H.S. up: Y.A. with Robert Metzger (left)

## About Me

I started my research at Prof. Kenichi Fukui's (One of the Nobel Prize laureates of chemistry in 1981) laboratory in Kyoto University where I got my Ph.D. by a thesis "A theoretical study of the vibronic coupling in molecules". After that I moved to the condensed matter theory group in the Electrotechnical Laboratory headed by Dr. Jun Kondo, with whom I have started my research career as a theoretical physicist. My academic interest covers wide range subjects both in condensed matter physics and chemical physics. In details, it includes non-equilibrium transport theory, strongly correlated electron system/many-body physics, theory of superconductivity, computational physics, charge migration in molecular aggregates and biological systems, theory of chemical reactions, and quantum chemistry. Currently, my research effort has been much focussed on non-equilibrium transport theory. The main achievements are the theory of inelastic electric current including the electro-phonon interaction, the fully self-consistent theory of electron and phonon (thereby heat) currents entangles by the electron-phonon interaction, the theory of the local heating and the electron-phonon coupling effect on the electric current shot noise. Some of the latest publications in these topics are listed below:

## (Main contributions)

1. Yoshihiro Asai, "Vibronic spectroscopy using current noise", Phys. Rev. B 91, 161402-1-4 (R) (2015): Rapid Communication.
2. Yoshihiro Asai, "Theory of zero-bias anomaly in low-temperature inelastic tunneling spectroscopy", Phys. Rev. B 86, 201405(R)-1-4 (2012): Rapid Communications.
3. Yoshihiro Asai, Hisao Nakamura, Joshua Hihath, Christopher Bruot, and Nongjian Tao, "Electron correlation enhancement of the diode property of asymmetric molecules", Phys. Rev. B 84, 115436-1-5 (2011).
4. Yoshihiro Asai, "Theory of local heating in single molecular bridge junctions", Phys. Rev. B, 84, 085436-1-7 (2011).
5. Yoshihiro Asai, "Nonequilibrium phonon effects on transport properties through atomic and molecular bridge junctions", Phys. Rev. B 78, 045434-1-24 (2008).
6. Yoshihiro Asai and Hidetoshi Fukuyama, "Theory of length dependent conductance of Hubbard chain", Phys. Rev. B 72, 085431-1-14 (2005).
7. Yoshihiro Asai, "Theory of inelastic electric current through single molecule", Phys. Rev. Lett. 93, 246102-1-4 (2004).

## (Collaborations: with theorists)

8. Hisao Nakamura and Yoshihiro Asai, "Competitive effects of oxygen vacancy formation and interfacial oxidation on an ultra-thin HfO<sub>2</sub>-based resistive switching memory: beyond filament and charge hopping models", Phys. Chem. Chem. Phys. 18, 8820-8826 (2016).
9. Xiaoliang Zhong, Ivan Rungger, Peter Zapol, Hisao Nakamura, Yoshihiro Asai and Olle Heinonen, "The effect of a Ta oxygen scavenger layer on HfO<sub>2</sub>-based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport", Phys. Chem. Chem. Phys. 18, 7502-7510 (2016).
10. Marius Bürkle, Thomas J. Hellmuth, Fabian Pauly, and Yoshihiro Asai, "First-principles calculation of the thermoelectric figure of merit for [2,2] paracyclophane-based single-molecule junctions", Phys. Rev. B, 91, 165419-1-8 (2015).
11. Hisao Nakamura, Tatsuhiko Ohto, Takao Ishida, and Yoshihiro Asai, "Thermoelectric Efficiency of Organometallic Complex Wires via Quantum Resonance Effect and Long-Range Electric Transport Property", J. Am. Chem. Soc. 135, 16545-16552 (2013).
12. Hisao Nakamura, Yoshihiro Asai, Joshua Hihath, Christopher Bruot, and Nongjian Tao, "Switch of Conducting Orbital by Bias-Induced Electronic Contact Asymmetry in a Bipyrimidinyl-biphenyl Diblock Molecule: Mechanism to Achieve a pn Directional Molecular Diode", J. Phys. Chem. C, 115, 19931-19938 (2011).
13. Tomomi Shimazaki and Yoshihiro Asai, "Theoretical study on the line shape of the inelastic tunneling spectroscopy", Phys. Rev. B 77, 115428-1-10 (2008).

(Collaborations with experimentalists)

14. Yueqi Li, Limin Xiang, Julio L. Palma, Yoshihiro Asai and Nongjian Tao, "Thermoelectric effect and its dependence on molecular length and sequence in single DNA molecules", Nature Communication, 7, 11294-1-8 (2016).
15. See Kei Lee, Marius Buerkle, Ryo Yamada, Yoshihiro Asai and Hirokazu Tada, "Thermoelectricity at the molecular scale: a large Seebeck effect in endohedral metallofullerenes", Nanoscale, 7, 20497 (2015).
16. Thomas Hines, Ismael Díez-Pérez, Hisao Nakamura, Tomomi Shimazaki, Yoshihiro Asai and Nongjian Tao, "Controlling Formation of Single-Molecule Junctions by Electrochemical Reduction of Diazonium Terminal Groups", J. Am. Chem. Soc. 135, 3319-3322 (2013): Communication.
17. See Kei Lee, Ryo Yamada, Shoji Tanaka, Gap Soo Chang, Yoshihiro Asai, and Hirokazu Tada, "Universal Temperature Crossover Behavior of Electrical Conductance in a Single Oligothiophene Molecular Wire", ACS Nano, 6, 5078-5082 (2012).
18. Kei-ichi Terada, Hisao Nakamura, Katsuhiko Kanaizuka, Masa-aki Haga, Yoshihiro Asai, and Takao Ishida, "Long Range Electron Transport of Ru-Center Multilayer Films via Stepping Stone Mechanism", ACS Nano, 6, 1988-1999 (2012).
19. Joshua Hihath, Christopher Bruot, Hisao Nakamura, Yoshihiro Asai, Ismael Díez-Pérez, Youngu Lee, Luping Yu, and Nongjian Tao, "Inelastic Transport and Low-Bias Rectification in a Single-Molecule Diode", ACS Nano, 5, 8331-8339 (2011).

The full list of my publication and more details will be described in following page. Currently, I am working with Dr. Marius Ernst Buerkle, Dr. Hisao Nakamura, and Dr. Jun-ichi Ozaki.



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